



FACULTAD DE
CIENCIAS QUÍMICAS

PHYSICAL CHEMISTRY II

COURSE GUIDE

BSc Chemistry

Academic Year 2023-2024



UNIVERSIDAD
COMPLUTENSE
MADRID



I.- IDENTIFICATION

COURSE NAME:	Physical Chemistry II
NUMBER OF CREDITS (ECTS):	12
CHARACTER:	Mandatory
SUBJECT:	Physical Chemistry
MODULE:	Fundamental
DEGREE:	Degree in Chemistry
SEMESTER/FOUR-MONTH PERIOD:	Yearly (second year)
DEPARTAMENT:	Physical Chemistry

RESPONSIBLE LECTURERS:

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Theory Group A	
1st semester Theory Seminar Tutoring	Professor: ANDRÉS GUERRERO MARTÍNEZ Department: Química Física Office: QA-249 e-mail: aguerrero@quim.ucm.es
2nd semester Theory Seminar Tutoring	Professor: LUIS GONZÁLEZ MACDOWELL Department: Química Física Office: QB-237 e-mail: lgtmac@quim.ucm.es
Theory Group B	
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2nd semester Theory Seminar Tutoring	Professor: ÁLVARO LOBATO FERNÁNDEZ Department: Química Física Office: QA-274 e-mail: a.lobato@ucm.es
Theory Group D	
1st semester Theory Seminar Tutoring	Professor: FERNANDO MARTÍNEZ PEDRERO Department: Química Física Office: QB-212C e-mail: fernandm@ucm.es
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Group	Semest.	Professor	e-mail	Office	Depar.
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II.- OBJECTIVES

■ GENERAL OBJECTIVE

In this course, the student will learn the fundamental concepts of thermodynamics, kinetics, surfaces, interfaces, polymers, and colloids that a graduate in Chemistry needs. The knowledge of chemical thermodynamics that the student has acquired in the first year will be complemented, and the study of statistical thermodynamics, kinetic theory, and transport properties will be addressed. Next, the kinetics of chemical reactions, surfaces and interfaces will be studied, including homogeneous and heterogeneous catalysis and electrode reactions. Finally, basic experimental concepts and techniques in the areas of polymers and colloids are included.



A general objective, of paramount importance, is to instill in the student a quantitative conception of Chemistry. In this sense, it is essential to convey the role that Physical Chemistry plays in Chemistry, not only as a set of concepts, theories, and experimental and calculation tools, capable of explaining the objects and phenomena that concern Chemistry, but also as the driving force behind chemical science and technology.

■ SPECIFIC OBJECTIVES

- To understand the thermodynamic potentials, in addition to the chemical potential and its use in the study of multicomponent systems.
- To understand the laws and properties of ideal and real solutions, including those formed by electrolytes.
- To learn the basic concepts and tools of statistical thermodynamics and their application in the case of non-interacting systems.
- To introduce students to the description of intermolecular forces by means of empirical potentials and their application in the calculation of the properties of interacting systems.
- To learn the fundamental concepts of the kinetic theory of gases and transport in condensed phases.
- To learn the fundamental aspects of chemical kinetics such as the relationship between the kinetic equation and the mechanism of complex reactions, theories of reaction rates, photochemistry, and homogeneous and heterogeneous catalysis.
- To introduce the student to the properties of surfaces and interfaces, such as surface tension and adsorption of gases on solids.
- To relate the properties of surfaces and interfaces to other phenomena, such as heterogeneous catalysis, at an elementary level.
- To understand the properties of equilibrium and transport in electrolyte solutions and the behaviour of the electrified interface, including the kinetics of electrode processes.
- To introduce the student to the basic experimental concepts and techniques in the area of polymers and colloids.

III.- PREVIOUS KNOWLEDGE AND RECOMENDATIONS

■ PREVIOUS KNOWLEDGE:

Contents of the basic subjects: *General Physics*, *Mathematics*, *General Chemistry*, *Basic Laboratory Operations* and *Computer Science Applied to Chemistry*; and of the subject *Physical Chemistry I* from the fundamental module.

■ RECOMENDATIONS:

It is recommended to review the contents of Thermodynamics and Chemical Kinetics acquired in previous courses.



IV.- CONTENTS

■ BRIEF DESCRIPTION OF THE CONTENTS:

Complements of thermodynamics. Statistical thermodynamics. Intermolecular forces. Real gases and condensed phases. Kinetic theory and transport phenomena. Chemical kinetics. Reaction mechanisms. Molecular approaches. Homogeneous catalysis. Surfaces and interfaces. Surface tension. Multicomponent systems. Physisorption and chemisorption. Electrode kinetics. Heterogeneous catalysis. Polymers and colloids. Synthesis and characterisation. Polymeric materials.

■ PROGRAM:

TOPIC I. Complements of Thermodynamics

Lesson 1: Thermodynamic potentials

Differential formulation of thermodynamics. Fundamental equation. Thermodynamic potentials (U , H , A , G). Maxwell's relations. Thermal coefficients. Equilibrium and spontaneity criteria.

Lesson 2: Multicomponent Systems

Partial molar quantities. Chemical potential. Gibbs-Duhem equation. Gibbs energy of a mixture. Chemical potential of an ideal gas. Chemical potential of a real gas: fugacity. Chemical potential of an ideal gas in a mixture of ideal gases. Thermodynamic quantities of mixing.

Lesson 3: Nonelectrolyte solutions

Ideal solutions: Raoult's law and Henry's law. Chemical potential of a component in an ideal solution. Real solutions. Chemical potential of a component in a real solution. Reference states. Activity and activity coefficient. Thermodynamics of mixing and excess functions.

Lesson 4: Electrolyte solutions

Electrolyte solutions. Electrochemical potential. Chemical potential of a component in an electrolyte solution. Reference states. Activity and activity coefficient. Debye-Hückel equation. Equilibrium electrochemistry.

Guided tutorials 1, 2 and 3

Laboratory 1: *Partial molar properties I.*

Laboratory 2: *Partial molar properties II.*

TOPIC II. Statistical Thermodynamics

Lesson 5: The partition function

Quantum-mechanical description of a microstate, degenerate states. Boltzmann's postulate. Canonical probability of a microstate. Canonical partition function. Relationship between the thermodynamic potentials and the canonical partition function. Examples of simple partition functions.

**Lesson 6: Non-interacting systems**

Molecular partition function: case of distinguishable and indistinguishable particles. Monoatomic gas: nuclear, electronic, and translational partition functions. Diatomic gas: rotational and vibrational partition functions. Energy, entropy and heat capacity of gases. High temperature limit, equipartition principle.

Lesson 7: Mixtures of non-interacting gases

Multicomponent partition function. Entropy of mixing. Chemical equilibrium. Equilibrium constants.

Lesson 8: Intermolecular forces. Real gases and condensed phases

Coulombic interactions. Multipole interactions: electric dipole. Induction and dispersion interactions. Empirical potentials: hard spheres, square well, Lennard-Jones. Classical partition function: configuration integral. Second virial coefficient. Van der Waals equation. Phase diagrams. Critical point.

Guided tutorials 4 and 5

Laboratory 3: Real gases I.

Laboratory 4: Real gases II.

TOPIC III. Kinetic theory and transport**Lesson 9: Kinetic theory of gases**

Maxwell-Boltzmann distribution of speeds. Most probable speed, mean speed and root mean square speed. Collision frequency and mean free path. Molecular flows. Diffusion and effusion. Transport properties: fluxes and gradients. Fick's law and self-diffusion coefficient of gases. Momentum transport, viscosity. Thermal conductivity.

Lesson 10: Transport in condensed phases

Mean square displacement and self-diffusion coefficient. Brownian motion. Viscosity and thermal conductivity. Transport in solids. Conductivity in electrolyte solutions. Ionic mobility. Kohlrausch's laws.

Guided tutorial 6

Laboratory 5: Conductimetry.

TOPIC IV. Chemical Kinetics**Lesson 11: Formal kinetics**

Advanced topics of formal kinetics. Experimental methods for the determination of reaction rates.

Lesson 12: Complex reactions

Reaction mechanisms: reversible, parallel, and consecutive reactions. Steady-state and rate-determining step approximations. Unimolecular reactions. Lindemann mechanism. Termolecular reactions. Chain reactions. Explosions.

**Lesson 13: Homogeneous catalysis**

General mechanism of catalysis. Acid-base catalysis. Autocatalysis.

Lesson 14: Photochemistry

Photochemical kinetics. Quantum yield. Quenching. Stern-Volmer equation. Photochemical reactions in the troposphere and the stratosphere.

Lesson 15: Theories of the reaction rates

Collision theory for rigid spheres: molecular collisions. Reactive cross-section. Line-of-centres model. Transition state theory: potential energy surfaces. Reaction path. Fundamental postulates and kinetic coefficient. Thermodynamic formulation.

Lesson 16: Kinetics of solution reactions

General properties of reactions in solution. Diffusion-controlled reactions. Transition state theory of reactions in solution.

Guided tutorials 7-9

Laboratory 6: *Spectrophotometry measurement of reaction kinetics.*

Laboratory 7: *Homogeneous catalysis.*

TOPIC V. Surfaces and interfaces**Lesson 17: Thermodynamics of the vapour-liquid interface**

Definition of interface and surface tension. Curved interfaces. Young-Laplace equation. Contact angle. Capillarity. Kelvin equation. Multicomponent systems. Excess surface properties. Gibbs isotherm. Types of solutes. Langmuir isotherm, monolayers, surface pressure, equation of state.

Lesson 18: Solid surfaces

Structure of a solid surface. Solid-gas interface. Adsorption. Physisorption and chemisorption. Fractional coverage. Experimental adsorption isotherms. BET model. Meaning of the C constant. Calculation of the specific surface area of a solid. Chemisorption. Langmuir isotherm. Other isotherms (Freundlich, Temkin). Isosteric heats. Heterogeneous catalysis.

Lesson 19: Processes at electrodes

Electrode-solution interface (electrified interfaces). Double-layer models: Helmholtz, Gouy-Chapman, Stern. Electrode kinetics. Overpotential. Exchange current density. Polarizable and non-polarizable electrodes.

Guided tutorials 10 and 11

Laboratory 8: *Surface tension of solutions. Gibbs equation. I*

Laboratory 9: *Surface tension of solutions. Gibbs equation. II*

Laboratory 10: *Adsorption isotherm.*

**TOPIC VI. Polymers and colloids****Lesson 20: Properties and synthesis of polymers**

Introduction, basic concepts. Polydispersity. Molecular weights. Flexibility and dimensions. Synthesis of polymers. Stepwise and chain polymerizations.

Lesson 21: Polymer solutions and characterization techniques

Thermodynamics of polymeric solutions. Θ temperature. Characterisation of polymers. Light scattering, viscosity, osmometry.

Lesson 22: Colloidal state and self-organization

Nature of the colloidal state. Micelles. Experimental determination of the critical micellar concentration.

Guided tutorial 12

Laboratory 11: *Viscosimetry for characterization of polymer solutions I.*

Laboratory 12: *Viscosimetry for characterization of polymer solutions II.*

Laboratory 13: *Determination of critical micellar concentrations.*

V.- COMPETENCES**■ GENERAL:**

The general competences of the degree, CG1, CG2, CG3, CG5, CG6, CG7, CG8, CG9, CG10, CG11, CG12 y CG13, developed in the fundamental module, CG-MF, and which are applicable in this course are the following:

- **CG1-MF1:** To recognize chemical processes in daily life.
- **CG2-MF1:** To relate Chemistry with other disciplines.
- **CG3-MF1:** To continue their studies in multidisciplinary areas.
- **CG5-MF1:** To demonstrate knowledge and understanding of the essential facts, concepts, principles, and theories related to the areas of Chemistry.
- **CG6-MF1:** To analyse and solve qualitative and quantitative problems.
- **CG7-MF1:** To recognize and analyse new problems and plan strategies to solve them.
- **CG8-MF1:** To consult and use scientific and technical information effectively.
- **CG9-MF1:** To demonstrate knowledge of laboratory materials and practical skills.
- **CG10-MF1:** To safely handle chemical materials.
- **CG10-MF2:** To recognize and assess the hazards in the use of chemicals and laboratory procedures.
- **CG11-MF1:** To handle standard chemical instrumentation.
- **CG12-MF1:** To interpret data from observations and measurements in the laboratory.



- **CG13-MF1:** To recognize and implement good scientific practices of measurement and experimentation.

■ **SPECIFIC:**

The specific competences of the subject Physical Chemistry that are applicable in this course are the following:

- **CE11-MFQF1:** To use the theoretical and experimental knowledge necessary to deal with the macroscopic behaviour of matter through the application of the principles of Chemical Thermodynamics, and its relationship with microscopic properties through the principles of Statistical Thermodynamics.
- **CE11-MFQF3:** To connect macroscopic properties and properties of individual atoms and molecules, including macromolecules, polymers, colloids, and other materials.
- **CE13-MFQF1:** To use the theoretical knowledge necessary to judge the changes associated with chemical reactions in terms of reaction mechanisms and rate equations, as well as the practical skills needed for the experimental quantification of these processes.
- **CE13-MFQF2:** To describe basic knowledge about electrochemical phenomena and their technological applications.

■ **TRANSVERSAL:**

The transversal competences of the degree, CT1, CT2, CT3, CT5, CT6, CT7, CT11 and CT12, developed in the fundamental module, CT-MF, and which are applicable in this course, are the following:

- **CT1-MF1:** To prepare and write scientific and technical reports.
- **CT2-MF1:** To cooperate with other students through teamwork.
- **CT3-MF1:** To apply critical and self-critical reasoning.
- **CT5-MF1:** To use chemical information, bibliographies, and specialized databases.
- **CT6-MF1:** To identify the importance of chemistry in the industrial, environmental, and social context.
- **CT7-MF1:** To use tools and computer programs for the treatment of experimental results.
- **CT11-MF1:** To develop autonomous learning.
- **CT12-MF1:** To recognize the current energy problem and its importance.
- **CT12-MF2:** To develop sensitivity to environmental issues.



VI. – LEARNING OUTCOMES

Once this course has been passed, in relation to the teachings included in the theoretical and practical program, the student should be able:

Lesson 1

1. To define the thermodynamic potentials A (Helmholtz energy) and G (Gibbs energy), together with those already known, such as U (internal energy) and H (enthalpy).
2. To apply the variations of the G energy to predict the spontaneity or equilibrium of processes at constant temperature and pressure.
3. To use Maxwell relations to deduce relationships between thermodynamic quantities.
4. To calculate the entropy variation of an ideal or van der Waals gas in any process.
5. To use the thermal coefficients to explain the relative volume changes at constant temperature or pressure of an ideal gas.
6. To explain under what conditions a system changes its Helmholtz energy, if that change is equal to the maximum work.

Lesson 2

7. To explain from a mathematical point of view the additivity of the partial molar properties in a mixture.
8. To define the chemical potential of a real gas using the reference state.
9. To explain that the variation of the chemical potential of one component of a mixture cannot be independent of the chemical potential of the rest of the components at constant temperature and pressure.

Lesson 3

10. To express the chemical potential of a component in solution as a function of the activities from different reference states.
11. To calculate activity coefficients of components in solution.
12. To interpret variations in the activity of solid and gaseous solutes and their environmental implications.
13. To evaluate equilibrium constants in solutions, in particular those of environmental interest, in terms of activity coefficients.
14. To calculate mixing and excess properties of solutions and to relate them to activity coefficients.

Lesson 4

15. To define the concept of electrolyte in solution.
16. To distinguish between activity and activity coefficient in real solutions and in electrolyte solutions.
17. To explain the Debye-Hückel theory in relation to the ionic strength of the medium.
18. To relate electrochemical processes to the concept of equilibrium in solution

Lesson 5

19. To apply the concepts of probability in the context of statistical thermodynamics.
20. To derive the Boltzmann distribution.



21. To explain the probabilistic nature of entropy.
22. To apply the Boltzmann distribution to systems of chemical interest.
23. To express thermodynamic properties from the canonical partition function.
24. To calculate the thermodynamic properties of simple systems from the molecular properties (partition function).

Lesson 6

25. To use the concept of non-interacting system and the resulting simplifications for the purpose of evaluation of the partition function.
26. To relate precise molecular properties to their corresponding partition functions and their effect on the thermodynamic properties of substances.
27. To apply the factorisation of partition functions in terms of separable molecular contributions.
28. To distinguish between quantum and classical statistics and to know the high-temperature relationship between them.

Lesson 7

29. To express the partition function of a mixture of non-interacting gases in terms of partition functions of pure species.
30. To describe the combinatorial origin of the entropy of mixing.
31. To explain the entropic and energetic factors that determine the equilibrium constants of a chemical reaction.
32. To express equilibrium constants of simple chemical reactions in terms of molecular properties.

Lesson 8

33. To name the types of intermolecular forces that a molecule can exhibit on the basis of its geometry.
34. To explain the distance dependence of the different intermolecular forces.
35. To compare the melting and boiling points of different substances on the basis of their intermolecular forces.
36. To describe the mathematical expressions for the most commonly used empirical potentials.
37. To calculate the equation of state of a real gas from the intermolecular potential and the configurational partition function for simple cases.
38. To describe and use the most frequently used semi-empirical equations of state.
39. To calculate the second virial coefficient from the interaction potential for simple cases.

Lesson 9

40. To explain the form of the Maxwell-Boltzmann speed and energy distribution functions and their dependence on temperature and molecular mass.
41. To calculate the mean speed, the most probable speed and the root mean square speed of a gas from the temperature and molecular mass.
42. To relate the energy equipartition theorem for an ideal gas to the equation of state.
43. To calculate the molecular collision frequency, total frequency and mean free path of pure gases and mixtures.



44. To apply the concepts of molecular diffusion and molecular effusion to simple systems.
45. To calculate the transport coefficients from the parameters of the kinetic theory.

Lesson 10

46. To relate the viscosity and thermal conductivity of real gases and fluids to the temperature and pressure of the system.
47. To define the concept of root mean square displacement and diffusion coefficient in real gases and dense fluids.
48. To apply the Einstein-Smoluchowski and Stokes-Einstein equations to determine the diffusion coefficient in dense fluids.
49. To analyse the concept of Brownian motion based on the phenomenon of diffusion in condensed phases.
50. To infer the phenomenon of diffusion in solids from the crystalline characteristics of the system.
51. To analyse the concept of molar conductance and conductivity to determine the mobility of ions in solution.
52. To apply Kohlrausch's laws in the determination of the limiting molar conductivity of an electrolyte solution.

Lesson 11

53. To apply the concepts of reaction rate, reaction order, elementary equation and molecularity in the context of a chemical reaction.
54. To determine the order of a reaction, its rate law and rate constant from experimental data for simple reactions.
55. To describe the different experimental methods for determining reaction rates.

Lesson 12

56. To derive a rate law from a reaction mechanism.
57. To determine the integrated rate equations for complex reactions: reversible, parallel, and consecutive reactions.
58. To use the steady-state and limiting-rate step approximations in a complex reaction.
59. To apply the Lindemann mechanism of unimolecular reactions.
60. To describe the different steps of straight-chain and branched-chain reactions, and to identify them in different examples.
61. To explain the mechanisms leading to explosive reactions.

Lesson 13

62. To explain the role played by a catalyst in a chemical reaction.
63. To explain homogeneous catalysis and, in particular, catalysis involving acids and bases.
64. To express the rate equation of the reaction including the terms in which the catalyst is involved.
65. To describe autocatalysis and its consequences.

Lesson 14

66. To calculate the rate of simple photochemical reactions.



67. To define the quantum yield of a given photophysical or photochemical process from the rate of the process and the intensity of the absorbed light.
68. To apply the Stern-Volmer equation to determine the collisional deactivation constant for a photophysical process.
69. To explain the role of photochemical steps and homogeneous catalysis in the reactions taking place in the troposphere and the stratosphere.

Lesson 15

70. To calculate the rate constant of bimolecular gas-phase reactions from molecular collisions.
71. To use potential energy surfaces and trajectories or reaction pathways to predict the transition state of a bimolecular reaction.
72. To calculate the rate constant of a gas-phase bimolecular reaction from the partition functions of the reactants and the activated complex.
73. To explain the prediction of the thermodynamic quantities of a reaction from the transition state theory.

Lesson 16

74. To describe the different types of reactions in solution.
75. To use the cell or cage effect to explain reactions in solution.
76. To use the diffusion coefficients to predict the rate constant of a diffusion-controlled reaction.
77. To describe the role of ionic strength in reactions in solution.

Lesson 17

78. To define the interfacial tension and, in particular, the surface tension.
79. To predict wetting based on a surface tension balance.
80. To explain the phenomena of capillary rise/depression and nucleation of a liquid in a vapour from the Young-Laplace equation.
81. To relate the excess surface concentration of a solute to its capacity to modify the surface tension of the solution.
82. To describe the thermodynamic behaviour of the vapour-liquid interface for solutions of surfactant solutes by means of surface equations of state.

Lesson 18

83. To describe the adsorption of a gas on the surface of a solid and to identify the differences between physisorption and chemisorption.
84. To recognise the different types of adsorption isotherms and to describe chemisorption using the Langmuir model and empirical equations (Temkin and Freundlich), and physisorption using the BET model for uniform non-porous surfaces.
85. To calculate the area of a solid surface and the enthalpy of adsorption from experimental data of the amount of adsorbed substance, using the BET model.
86. To calculate the isosteric enthalpy of adsorption from suitable experimental data.
87. To relate chemisorption to the processes of heterogeneous catalysis.

**Lesson 19**

88. To describe the different models for the electrical double layer at an electrified interface.
89. To distinguish the behaviour of polarisable and non-polarisable electrodes.
90. To apply the Butler-Volmer equation to determine the current density from the overpotential.

Lesson 20

91. To recognise basic concepts specific to polymers, and their classification.
92. To explain the implications of polydispersity, and to calculate molecular weight averages.
93. To explain the concepts of flexibility and stiffness of chains, and to calculate average dimensions.
94. To distinguish the different mechanisms of synthesis of linear polymers, and to calculate their reaction rates.
95. To calculate the average molecular weights as a function of time in step polymerisations.
96. To calculate the average molecular weights and masses of polymer obtained in chain polymerisations.

Lesson 21

97. To handle the Flory-Huggins theory to determine the possible formation of polymer solutions.
98. To relate the "theta" temperature to solvent quality and the Flory interaction parameter.
99. To use osmotic pressure measurements to determine number-average molecular weights.
100. To use light scattering data to calculate weight-average molecular weights.
101. To experimentally determine intrinsic viscosities to calculate the viscous-average molecular weight.

Lesson 22

102. To describe the concepts of micelles and colloids, their types and classification.
103. To experimentally determine the critical micellar concentration of a surfactant.



VII. – WORKING HOURS AND DISTRIBUTION BY ACTIVITY

Activity	Presential (hours)	Autonomous work (hours)	Credits
Theoretical classes	48	77	5
Seminars	24	11	1,4
Tutorials / Directed work	12	18	1,2
Laboratory practices	42	45,5	3,5
Preparation of reports and exams	6	16,5	0,9
Total	132	168	12

VIII.- METHODOLOGY

The contents of the course are presented to the students in face-to-face classes, divided into two types:

Face-to-face theory lectures will be given to the whole group in order to introduce the fundamental contents of the subject. At the end of the subject a brief summary of the most relevant concepts will be made, and new objectives will be proposed that will allow the interrelation of contents already studied with those of the rest of the subject and with other related subjects. During the exposition of contents, problems that exemplify the concepts developed or that serve as an introduction to new contents will be proposed. To facilitate the student's monitoring of the face-to-face lectures, the necessary teaching material will be provided, either as photocopies or preferentially through the Virtual Campus.

In the face-to-face seminars, exercises and questions that exemplify the contents developed in the theory lectures will be solved. Periodically the student will be provided with a list of these problems/exercises with the aim of trying to solve them before the classes, which will include in some cases the search of scientific sources. The process of solving these problems will be carried out by means of different methods. Some exercises will be collected by the teacher for evaluation. These theory and seminar classes and the work they involve develop the general competences CG6-MF1, CG7-MF1 and CG8-MF1, and the transversal competences CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1 and CT7-MF1.

During the development of the syllabus, both in the theory classes and in the seminars, the student will acquire the knowledge and experience necessary to accomplish all the specific competences to be covered, CE11-MFQF1, CE11-MFQF3, CE13-MFQF1 and CE13-MFQF2, and the transversal competence CT11-MF1. In addition, during the development of the sessions, special emphasis will be placed on relating the aspects studied with other disciplines and chemical phenomena in daily life, as well as on their multidisciplinary nature, which will satisfy the general competences CG1-MF1, CG2-MF1 and CG3-MF1, and the transversal competences CT12-MF1 and CT12-MF2.

In the tutorial classes, exercises will be proposed and solved both on subjects directly related to the theoretical contents and on more applied subjects. As a complement to the



personal work carried out by the student, and to promote the development of group work, topics for the preparation and presentation of work may be proposed. All these activities will allow students to put into practice their skills in obtaining information, developing skills related to the critical use of bibliographic information and databases and teamwork (CT2-MF1, CT3-MF1 and CT5-MF1). In addition, each working group will be able to evaluate, anonymously, the topic developed by another group, in a similar way to the peer review of scientific publications, which will develop the critical and self-critical sense covered in the transversal competence CT3-MF1. The assessment process will help students to develop their ability to critically analyse scientific work, and to be able to correct in their own work any defects they find in the work they assess.

The professor will schedule tutorials available for individual students who wish to resolve any doubts that may arise during the study. These tutorials will be held in person at the times indicated by each professor or, exceptionally, virtually.

The Virtual Campus will be used to allow a fluid communication between professors and students and as an instrument to make available to the students the material to be used in the theoretical and problem classes. It may also be used as a forum in which to present some complementary topics whose content, although important to the subject as a whole, is not considered appropriate to be presented in face-to-face classes. Finally, this tool will allow self-assessment exercises to be carried out by means of automatically corrected multiple-choice objective tests, which will show both the teacher and the student which concepts require more work for their learning.

A laboratory will be conducted throughout the course with topics directly related to the contents of the course. This laboratory will consist of experimental practices, where the general competences will be specifically developed (CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG12-MF1 y CG13-MF1). These practices also require the use of calculations and theoretical tools which will contribute to the development of specific competences (CE11-MFQF1, CE11-MFQF3, CE13-MFQF1 y CE13-MFQF2). The student will present individual or small group scientific reports of some of the practices carried out. In these reports, the student will describe the work done, including a critical discussion about the methods employed and the quality of the results obtained. (CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT7-MF1).

IX.- BIBLIOGRAPHY

■ **BASIC:**

- *Química Física*, P. Atkins, J. de Paula, 8ª Edición, Editorial Médica Panamericana, Buenos Aires, 2008.
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<https://biblioteca.ucm.es/quimica-fisica>
<https://www-medicapanamericana-com.bucm.idm.oclc.org/VisorEbookV2/Ebook/9789500694988?token=852344e8-effc-44de-a8f3-4a31d6982771#{%22Pagina%22:%221%22,%22Vista%22:%22Indice%22,%22Búsqueda%22:%22%22}}>
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■ ADDITIONAL:

- *Química Física*, P. Reid, T. Engel, Pearson Addison Wesley, Madrid, 2006.
Available online from the UCM-Ingebooks web page:
https://www.ingebook.com/ib/NPcd/IB_BooksVis?cod_primaria=1000187&codigo_libro=1292
- *Principios de Fisicoquímica*, I.N. Levine, 6^a Edición, McGraw Hill/Interamericana, México, 2014. 5th Edition (in Spanish) available online from the UCM-Ingebooks web page:
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- *Química Física*, Volumes I and II. J. Bertrán Rusca and J. Núñez Delgado (coord.). Ariel Ciencia, 2002.
- *Physical Chemistry*, R. S. Berry, S. A. Rice, and J. Ross, 2nd Edition, Oxford University Press, New York, 2000.
- *Physical Chemistry: A Molecular Approach*, D. A. McQuarrie y J. D. Simon, University Science Book, 1997.
- *Molecular driving forces*, K. A. Dill, S. Bromberg, 2nd Edition, Garland Science, New York, 2010.
- *Problemas de Química Física*, J. Bertrán Rusca and J. Núñez Delgado (coords.). Delta Publicaciones, 2007.

X.- GRADING RULES

The student's academic performance and the final grade of the course will be weighted according to the following percentages, which will be maintained in all the examination calls. In general, to pass the course, it will be necessary to achieve a minimum grade of 5 out of 10 points in the total computation of all the evaluated activities.

■ WRITTEN EXAMS:

65%

Ordinary call: two mid-term exams and a final exam, common to all groups, will be held.

To pass this call through mid-term exams it will be necessary:

- a) To obtain a minimum grade of 10 out of 20 in the sum of the two mid-term exams.
- b) To have at least 4 out of 10 marks on both mid-term exams.
- c) That the total grade weighted with the rest of the activities is at least 5 out of 10.

Students who pass this call by mid-term, i.e., who meet the above conditions, need not take the final exam. The remaining students will have to either take the exam of the subject of the partial not passed (partial-final), or of the full course, in the final exam of the ordinary call. To be able to opt for the partial-final exam modality in the ordinary exam, the student must have obtained a minimum grade of 5 in the partial of which



he/she is not examined and a grade higher than 2 out of 10 in the partial of which he/she is examined.

The grades of the partial exams will be published within a maximum period of 20 days from the date of the exams, though in the second one the period may be shorter depending on the date of the final exam. In any case, the minimum period of seven days between the publication of the grades and the date of the final exam of the course will be respected.

All midterm, final and partial-final exams will consist of questions and problems on the contents of the course, both theoretical classes and seminars, tutorials, and laboratories. In the exam of the ordinary call, the students who take only a partial exam, because they have passed the other one, will take an exam equivalent, in number of questions and time, to those who take the final exam.

In the extraordinary call, a single final exam like the one taken in the ordinary call will be taken. Those who do not pass the course in the ordinary exam will have to take the entire syllabus.

In any case, the minimum grade of the final exam required to pass the subject, both in the ordinary and extraordinary calls, is 4 out of 10.

Competences assessed:

CG1-MF1, CG2-MF1, CG3-MF1, CG5-MF1, CG6-MF1, CG7-MF1, and CG8-MF1
CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT7-MF1, CT11-MF1, CT12-MF1, and CT12-MF2
CE11-MFQF1, CE11-MFQF3, CE13-MFQF1, and CE13-MFQF2

■ **HOMEWORK:**

10%

The evaluation of the individual learning work done by the student will be carried out considering the following factors:

- Skills of the student in the resolution of the proposed problems and exercises, which will be collected periodically either in face-to-face lectures or through the Virtual Campus.
- Assessment of the work done in face-to-face seminar lectures.
- Assessment of the work proposed in the programmed tutorials and carried out individually or in groups by the students.

For the homework grade to add up, students will need to achieve at least 5 out of 10 marks in this task.

Competences evaluated:

CG1-MF1, CG2-MF1, CG3-MF1, CG5-MF1, CG6-MF1, CG7-MF1, and CG8-MF1
CE11-MFQF1, CE11-MFQF3, CE13-MFQF1, and CE13-MFQF2
CT2-MF1, CT3-MF1, CT5-MF1, CT6-MF1, and CT11-MF1

■ **LABORATORY:**

25%

The students will develop in reduced groups throughout the course a series of laboratory practices of experimental character as well as of calculation and use of theoretical tools, being the attendance to these practices **mandatory**. The general attitude of the students in the laboratory, their work during the practical sessions, the



acquisition by the student of theoretical and practical skills, as well as the skill in the use of the experimental equipment and in the handling of computer packages for data processing and molecular modelling will be graded. Students will have to fill an individual laboratory notebook, which will be subject to grading and marking each semester. Additionally, during the development of the laboratory, the professors will order exercises or elaboration of data that will be delivered in the established term and will count for the evaluation of the practical session. Both the laboratory notebook and the exercises will be marked, and therefore the student must deliver them by the scheduled deadlines.

The evaluation of the face-to-face activity and reports will constitute 70% of the laboratory qualification. The remaining 30% of the marks will correspond to a specific exam once the laboratory is finished, being required that the grade in this exam is equal or higher than 4. The student will not pass the laboratory if the individual grades of 4 or more practices is less than 5 out of 10. The minimum global grade of the laboratory necessary to compensate with the rest of the evaluations (exams, homework) will be 4 out of 10.

Those students who have not passed the laboratory in the ordinary call, could take a laboratory exam in the extraordinary call, but only if they have passed the written exams of the course, they have assisted to all the laboratory sessions, and delivered all the laboratory reports for grading. Moreover, in the extraordinary call these students must deliver a new set of laboratory reports for those practices which they got with a grade less than 5 out of 10.

In those cases in which a student fails the course, but has passed the face-to-face laboratory part, the grade of the laboratory activity and reports will be maintained for a maximum of two consecutive academic years following that in which he/she passed those activities. In addition, the student **will have to take the exam of the laboratory contents** in the ordinary or extraordinary call to pass the course.

Competences assessed:

CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG12-MF1, and CG13-MF1
CE11-MFQF1, CE11-MFQF3, CE13-MFQF1, and CE13-MFQF2
CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, and CT7-MF1

■ ATTENDANCE AND ACTIVE PARTICIPATION IN CLASSES:

Attendance at all face-to-face activities is mandatory. **The student's attitude and active participation** in all teaching activities will be positively valued in the final grade.

**ACTIVITY PLANNING - CHRONOGRAM**

TOPIC	ACTIVITY	HOURS	GROUPS	START	END
I. Complements of Thermodynamics	Theory lectures	9	1	1 st week	6 th week
	Problem solving lectures	5	1		
	Scheduled tutoring	3	1		
	Laboratory	6	4		
II. Statistical Thermodynamics	Theory lectures	8	1	6 th week	11 th week
	Problem solving lectures	5	1		
	Scheduled tutoring	2	1		
	Laboratory	6	4		
III. Kinetic Theory and Transport	Theory lectures	6	1	11 th week	14 th week
	Problem solving lectures	3	1		
	Scheduled tutoring	1	1		
	Laboratory	3	4		
IV. Chemical Kinetics	Theory lectures	11	1	15 th week	21 st week
	Problem solving lectures	6	1		
	Scheduled tutoring	3	1		
	Laboratory	7	4		
V. Surfaces and Interfaces	Theory lectures	9	1	21 st week	26 th week
	Problem solving lectures	3	1		
	Scheduled tutoring	2	1		
	Laboratory	9,5	4		
VI. Polymers and Colloids	Theory lectures	5	1	26 th week	28 th week
	Problem solving lectures	2	1		
	Scheduled tutoring	1	1		
	Laboratory	10,5	4		



SUMMARY OF ACTIVITIES AND TASKS

PLAN FOR EACH THEORY GROUP

Teaching activity	Associated competences	Teacher Activity	Student Activity	Evaluation procedure	P	NP	Total	C
Theory face-to-face lectures	CG1-MF1, CG2-MF1, CG3-MF1, CG6-MF1, CG7-MF1, CG8-MF1, CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT7-MF1, CT11-MF1, CT12-MF1, CT12-MF2, CE11-MFQF1, CE11-MFQF3, CE13-MFQF1, CE13-MFQF2	Presentation of theoretical concepts and posing of questions and new objectives.	Taking notes. Resolution of questions. Development of the new objectives. Formulation of questions and doubts.	Grading of the answers given to questions related to the theoretical concepts.	48	77	125	10%
Face-to-face seminars		Application of the theory to solving numerical exercises and problems. Raising new questions.	Resolution of numerical exercises, problems, and questions. Formulation of questions and doubts.	Grading of the answers (approach and result) given for the resolution of numerical exercises and problems.	24	11	35	
Tutorials		Direction and supervision of the student's study and activities. Raising questions. Resolving doubts.	Discussion with the professor on the conceptual and methodological difficulties encountered when studying the subject. Raising questions and answering those proposed by the professor.	No evaluable				
Scheduled tutorials		Proposal and critical assessment of work. Presentation and proposal of new objectives.	Cooperation with classmates in the preparation of work. Critical analysis of the work of other groups. Oral presentation of corrected work. Formulation of questions and doubts.	Assessment of the work, the analyses carried out and the presentation.	12	18	30	



Course Guide:

Physical Chemistry II



Teaching activity	Associated competences	Teacher activity	Student activity	Evaluation procedure	P	NP	Total	C
Laboratory	CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG12-MF1, CG13-MF1, CT1-MF1, CT2-MF2, CT3-MF3, CT5-MF1, CT7-MF1, CE11-MFQF1, CE11-MFQF3, CE13-MFQF1, CE13-MFQF2	Application of theoretical content to practical problems. Development of experimental and numerical calculation skills. Obtaining and processing experimental data.	Preparation, completion, and study of the proposed contents. Preparation of a report on the practical work carried out.	Assessment of the work carried out and the results obtained. Grading of the internship report submitted. Assessment of the skills and knowledge acquired.	42	45,5	87,5	25%
Exams		Proposal, invigilation, and correction of the exam. Grading of the student.	Preparation and realisation.	Correction and assessment of examinations.	6	16,5	22,5	65%
P: Face-to-face; NP: non face-to-face (autonomous work); C: Mark								

